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Software Requirements, Design, and Verification and Validation for the FEHM Application—A Finite-element Heat- and Mass-transfer Code

by

Zora V. Dash, Bruce A. Robinson, and George A. Zyvoloski

ABSTRACT

The requirements, design, and verification and validation of the software used in the FEHM application, a finite-element heat- and mass-transfer computer code that can simulate nonisothermal multiphase multicomponent flow in porous media, are described. The use of this code is applicable to natural-state studies of geothermal systems and groundwater flow. A primary use of the FEHM application will be to assist in the understanding of flow fields and mass transport in the saturated and unsaturated zones below the proposed Yucca Mountain nuclear waste repository in Nevada. Chapter I describes the software requirements specification for the FEHM application, including the functional and external interface requirements. This specification motivates the software design, discussed in Chapter II, which covers functional requirements, input/output files and associated variables, and error and warning conditions with their associated messages. Chapter III, “Verification and Validation Plan,” outlines the manner in which rigorous and complete testing of the model is to be carried out. Whenever possible, the testing will be against known analytical solutions of the same problem, or for more complex test cases for which no analytical solution exists, the code will be benchmarked against the results of other numerical models. The test cases to be performed are detailed and acceptance criteria that must be satisfied are listed. Chapter IV discusses those test cases and describes the results. The cases covered include tests of separate model components, such as the thermodynamic functions or heat conduction, and tests of a more complex nature, such as dry-out of a partially saturated medium, fracture transport with matrix diffusion, multisolute transport with chemical reaction, and three-dimensional radionuclide transport with decay chain. The test of the DOE Code Comparison Project, Problem Five, Case A, which verifies that FEHM has correctly implemented heat and mass transfer and phase partitioning, is also covered.

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1.0 PURPOSE

The FEHM application consists of a finite-element-based numerical simulator of nonisothermal, multiphase, multicomponent flow and solute transport in porous media. The FEHM code will be used for parameter sensitivity studies in the design and specification of field tracer and flow experiments and the interpretation of those field experiments. In addition, it will be used for field-scale simulations of radionuclide migration in the saturated and unsaturated zones below the proposed nuclear waste repository at Yucca Mountain, Nevada.

This document includes the following four main chapters:

- **I. Software Requirements Specification.** This chapter documents the functional requirements for the FEHM application that are used in designing the application. Subsequent baseline studies (described in Chapter IV, "Verification and Validation Report") are used to verify that the application fully implements these requirements.
- **II. Software Design.** The design of the FEHM software is described, including functional requirements, input/output files and associated variables, and error and warning conditions with associated messages.
- **III. Verification and Validation Plan.** The Verification and Validation effort tests the options and features of the FEHM application to verify that the requirements specified in Chapter I, "Software Requirements Specification," are satisfied. The approach is to consist of rigorous and complete testing of the model, whenever possible, against known analytical solutions of the same problem or, for more complex test cases for which no analytical solution exists, of benchmarking the code against the results of other numerical models. This chapter details the test cases to be performed, many of which were developed for prior versions of FEHM (Zyvoloski et al. 1992; Zyvoloski and Dash 1991a, 1991b), and lists the acceptance criteria that must be satisfied.
- **IV. Verification and Validation Report.** This chapter discusses the test cases described in "Verification and Validation Plan" and details the results of those tests.

2.0 DEFINITIONS AND ACRONYMS

2.1 Definitions

FEHM: Finite-element heat- and mass-transfer code (Zyvoloski et al. 1988).

FEHMN: an earlier verion of FEHM designed specifically for the Yucca Mountain Site Characterization Project. Both versions are now equivalent, and the use of FEHMN has been dropped.

2.2 Acronyms

DOE - U. S. Department of Energy

DKM - double-porosity/double-permeability method

ECM - equivalent continuum method

LANL - Los Alamos National Laboratory

LU - lower-upper

USGS - United States Geological Survey

V&V - verification and validation

YMP - Yucca Mountain Site Characterization Project

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